

Molecular orbitals and the principle of quantum superposition.

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Note that the energy of the original atomic orbitals and the energy of the formed molecular orbitals are different. This is precisely why molecular orbitals contradict quantum mechanics.

Let's remember chemistry. According to the molecular orbital method, the wave function is represented by a linear combination of overlapping atomic orbitals:

$$\psi = C_1\psi_1 + C_2\psi_2$$

where ψ_1 , ψ_2 are the wave functions of atomic orbitals.

Next, we consider two quantum states (really existing ones) described by the wave functions ψ_1 and ψ_2 . From the principle of quantum superposition it follows that the linear combination ($\psi_3 = C_1\psi_1 + C_2\psi_2$) will be the third quantum state (really existing), which will be described by the wave function ψ_3 .

This means that measuring some physical quantity E in the state $|\psi_1\rangle$ will give E_1 , and measuring E in the state $|\psi_2\rangle$ will give E_2 .

When measuring E in the third quantum state $|\psi_3\rangle$, the quantum system will sometimes take the value E_1 , and sometimes the value E_2 (with a certain frequency). That is, in the third quantum state ($\psi_3 = C_1\psi_1 + C_2\psi_2$) we will have a discrete set of values of a physical quantity.

This means that molecular orbitals cannot have an energy different from the original atomic orbitals.

In fact, the classical definition of molecular orbitals contradicts the principle of quantum superposition, that is, it is erroneous.

Principle of quantum superposition:

“...Suppose that in a state with a wave function $\psi_1(q)$ some measurement leads with certainty to a certain result - result 1, and in a state $\psi_2(q)$ - to result 2. Then it is assumed that any function of the form $C_1\psi_1 + C_2\psi_2$ (C_1 , C_2 - constants), describes a state in which the same measurement will give either result 1 or result 2...

These statements constitute the content of the so-called principle of superposition of states - the main positive principle of quantum mechanics. It follows from it, in particular, that all equations satisfied by the wave functions must be linear in ψ ...” (Landau L. D., Lifshits E. M. Theoretical physics in 10 volumes. Volume 3. Quantum mechanics. Fourth edition. M.: Nauka, 1989, pp. 20 - 21).